AN ALTERNATIVE SOFTWARE SOLUTION FOR GC×GC-MS DATA PROCESSING

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Comprehensive two-dimensional gas chromatography (GC×GC) coupled to mass spectrometry (MS) is a powerful tool for the consideration of challenging (semi) volatile organic compound ((S)VOC) mixtures. Targeted and non-targeted approaches have been applied to a large variety of matrices, further pushing hyphenation of GC×GC to high resolution Time-of-Flight (HRTOF) MS. The progress of the technical aspects comes with an increase of data complexity. However, only a limited number of software are available to handle GC×GC data although data treatment and interpretation are essential steps of reliable analysis. Available GC×GC data processing software are licensed, oftentimes require high expertise by the user due to their complexity, and their use can be labor-intense and time-consuming.

A new software called Canvas by J&X Technologies was applied for the analysis of the Grob mix standard solution. The software offers the option of single-chromatogram interpretation, one-to-one comparison of two chromatograms and batch analysis. Replicate injections were used to evaluate the software-integrated alignment tool. Satisfying results were achieved for the match factor and similar 2D-retention-shifts were reported as obtained by manual alignment. Simple automated retention indices calculation can be integrated. Limitations were though that the different tools cannot be combined and features such as normalization of the area are not available yet. Regarding all steps, it was found that the data processing time was very fast compared to other GC×GC software. Similar as in other programs library search for compound identification can be conducted. Peak tables including information such as integrated peak area, peak height, retention times, peak width etc. can be generated and exported as .csv files for further statistical treatment. Within the framework of this study, it could be demonstrated that the Canvas software is an interesting alternative for GC×GC MS data processing. However, further testing on more complex samples and bigger data sets needs to be conducted to fully assess its potential.